D-Alanine, N-(2-chlorobenzoyl)-, hexyl ester

Inchi: InChI=1S/C16H22ClNO3/c1-3-4-5-8-11-21-16(20)12(2)18-15(19)13-9-6-7-10-14(13)17/h
InchiKey: YVDQZPIEILVIER-UHFFFAOYSA-N
Formula: C16H22ClNO3
SMILES: CCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 311.80

Physical Properties

Property code	Value	Unit	Source
gf	-101.20	kJ/mol	Joback Method
hf	-473.44	kJ/mol	Joback Method
hfus	41.01	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.582		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	814.46	K	Joback Method
tc	1025.06	K	Joback Method
tf	498.69	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.43	J/mol×K	814.46	Joback Method
cpg	717.27	J/mol×K	849.56	Joback Method
cpg	730.09	J/mol×K	884.66	Joback Method
cpg	741.93	J/mol×K	919.76	Joback Method
cpg	752.81	J/mol×K	954.86	Joback Method
cpg	762.77	J/mol×K	989.96	Joback Method
cpg	771.84	J/mol×K	1025.06	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume